

Full Text

AN 1990:4003 CAPLUS

DN 112:4003

TI An algorithm for multiple alignment of protein sequences

AU Park, Kiejung; Sheen, Joonho; Park, Chankyu

CS Dep. Biol. Sci. Eng., Korea Adv. Inst. Sci. Technol., Seoul, 150, S. Korea

SO Han'guk Saenghwa Hakhoechi (1989), 22(3), 346.54

CODEN: KBCJAK; ISSN: 0368.4881

DT Journal

LA Korean

AB One application of computers in mol. biol. has been for comparing a large no. of mol. sequences in very short time. For this purpose, a new algorithm is proposed which differs in several aspects from other approaches. This algorithm, called MAlign, is designed to seek global homol. by introducing an effective way to make simultaneous comparisons among test sequences. One problem in previous algorithms which were limited in its ability to compare sequences simultaneously has been solved by introducing intermediate consensus or compacted sequences and including them for comparison. In addn., a homol. vector concept was applied to provide uniform representation for each intermediate, which makes global comparison easier. Several test results indicate that high homol. values obtained from pairwise alignment are maintained after multiple alignment of those sequences, which is more apparent in higher homol. values. Sample alignment results using this approach for three different copper-binding proteins as well as bacterial signaling proteins are presented.

Full Text

AN 1995:228028 CAPLUS

DN 122:27196

TI Multiple protein structure alignment

AU Taylor, William R.; Flores, Tomas P.; Orengo, Christine A.

CS Lab. Mathematical Biol., Natl. Inst. Med. Res., London, NW7 1AA, UK

SO Protein Science (1994), 3(10), 1858.70

CODEN: PRCIEI; ISSN: 0961.8368

PB Cambridge University Press

DT Journal

LA English

AB A method was developed to compare protein, e.g., IgG, structures and to combine them into a multiple structure consensus. Previous methods of multiple structure comparison have only concatenated pairwise alignments or produced a consensus structure by averaging coordinate sets. The current method is a fusion of the fast structure comparison program SSAP and the multiple sequence alignment program MULTAL. As in MULTAL, structures are progressively combined, producing intermediate consensus structures that are compared directly to each other and all remaining single structures. This leads to a hierarchic "condensation", continually evaluated in the light of the emerging conserved core regions. Following the SSAP approach, all interat. vectors were retained with well.conservd regions distinguished by coherent vector bundles (the structural equiv. of a conserved sequence position). Each bundle of vectors is summarized by a resultant, whereas vector coherence is captured in an error term, which is the only distinction between conserved and variable positions. Resultant vectors are used directly in the comparison, which is weighted by their error values, giving greater importance to the matching of conserved positions. The resultant vectors and their errors can also be used directly in mol. modeling. Applications of the method were assessed by the quality of the resulting sequence alignments, phylogenetic tree construction, and data bank scanning with the consensus. Visual assessment of the structural superpositions and consensus structure for various well.characterized families confirmed that the consensus had identified a reasonable core.

Full Text

AN 940876846 JICST.EPlus

TI Substructure Search and Alignment Algorithms for Three-Dimensional Protein Structures.

AU AKUTSU T

CS Gunma Univ., Gunma, JPN

SO Joho Shori Gakkai Kenkyu Hokoku, (1994) vol. 94, no. 82(AL.41), pp. 1.8.

Journal Code: Z0031B (Fig. 1, Tbl. 2, Ref. 22)

ISSN: 0919.6072

CY Japan

DT Journal; Article

LA English

STA New

AB This paper presents two practical algorithms for pattern matching of 3D protein structures: a hashing technique for quick substructure search and an alignment algorithm for 3D structures. In both algorithms, protein structures are treated as point sequences. In the hashing technique, for each fixed-length sequence, a hash vector is computed, where the distance between two hash vectors is small if two sequences are similar. In the alignment algorithm, a correspondence of points between two sequences is computed. In each algorithm, a theoretical proof for the quality of outputs is given. Moreover, experimental results show that both algorithms are effective. (author abst.)

L5 ANSWER 23 OF 78 MEDLINE

Full Text

AN 91332920 MEDLINE

DN 91332920 PubMed ID: 1908023

TI Average values of a dissimilarity measure not requiring **sequence alignment** are twice the averages of conventional mismatch counts requiring **sequence alignment** for a variety of **computer.generated** model systems.

AU Blaisdell B E

CS Department of Mathematics, Stanford University, CA 94305.

SO JOURNAL OF MOLECULAR EVOLUTION, (1991 Jun) 32 (6) 521.8.

Journal code: 0360051. ISSN: 0022.2844.

CY United States

DT Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals

EM 199109ED Entered STN: 19911006

Last Updated on STN: 19911006

Entered Medline: 19910917

AB A measure of **sequence** similarity, d_t , not requiring prior **sequence alignment** gave correct results for a variety of **computer.generated** model **sequences** without and with gaps for all degrees of substitution, s . Measure d was the squared Euclidean distance between **vectors** of counts of t -tuplets of characters in the two **sequences**. In models without gaps and without Needleman.Wunsch **alignment**, average d was very closely equal to twice average conventional mismatch counts, m . In these models one of each of the conditions on the Jukes.Cantor model was violated in turn: (1) both descendant lineages receive the same number of substitutions, (2) all sites are equally likely to be substituted, (3) all different replacement characters are equally likely to be chosen, and (4) all original characters are equally likely to be substituted. In Jukes.Cantor models with gaps Needleman.Wunsch **alignment** was necessarily performed, a procedure that generally produced incorrect values of m . For these models average d was found to be very closely equal to twice the average m estimated from the known value of s using the inverted Jukes.Cantor formula.

Full Text

RESERVED.

AN 2003.0168454 PASCAL

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TIEN Application of Max.plus algebra to biological **sequence** comparisons

Max.plus algebras

AU COMET J..P.

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INRIA, Rocquencourt, France; CNRS, IRCCyN, Nantes, France; CNRS, LIAFA,
Paris, France; Universite Paris 7, LIAFA, Paris, France

SO Theoretical computer science, (2003), 293(1), 189.217, 28 refs.

ISSN: 0304.3975 CODEN: TCSCDI

DT Journal

BL Analytic

CY Netherlands

LA English

AV INIST.17243, 354000107253650100

AB The classical **algorithms** to align two biological **sequences**

(Needleman and Wunsch and Smith and Waterman **algorithms**) can be seen as

a **sequence** of elementary operations in (max, +) algebra: each line

(viewed as a vector) of the dynamic programming table of the

alignment algorithms can be deduced by a (max, +) multiplication of

the previous line by a matrix. Taking into account the properties of

these matrices there are only a finite number of nonproportional

vectors. The use of this algebra allows one to imagine a faster

equivalent **algorithm**. One can construct an automaton and afterwards

skim through the **sequence** databank with this automaton in linear time.

Unfortunately, the size of the automaton prevents using this approach for

comparing global proteins. However, biologists frequently face the

problem of comparing one short string against many others **sequences**. In

that case this automaton version of dynamic programming results in a new

algorithm which works faster than the classical **algorithm**.

LS ANSWER 35 OF 78 MEDLINE

Full Text

AN 2002331987 MEDLINE

DN 22069937 PubMed ID: 12075023

TI SST: an algorithm for finding near.exact sequence matches in time proportional to the logarithm of the database size.

AU Giladi Eldar; Walker Michael G; Wang James Z; Volkmuth Wayne

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SO BIOINFORMATICS, (2002 Jun) 18 (6) 873.7.

Journal code: 9808944. ISSN: 1367.4803.

CY England: United Kingdom

DT Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals

EM 200301

ED Entered STN: 20020621

Last Updated on STN: 20030128

Entered Medline: 20030127

AB MOTIVATION: Searches for near exact sequence matches are performed frequently in large.scale sequencing projects and in comparative genomics. The time and cost of performing these large.scale sequence.similarity searches is prohibitive using even the fastest of the extant algorithms. Faster algorithms are desired. RESULTS: We have developed an algorithm, called SST (Sequence Search Tree), that searches a database of DNA sequences for near.exact matches, in time proportional to thelogarithm of the database size n. In SST, we partition each sequence into fragments of fixed length called 'windows' using multiple offsets. Each window is mapped into a vector of dimension 4(k) which contains the frequency of occurrence of its component k.tuples, with k a parameter typically in the range 4.6. Then we create a tree.structured index of the windows in vector space, with tree.structured vector quantization (TSVQ). We identify the nearest neighbors of a query sequence by partitioning the query into windows and searching the tree.structured index for nearest.neighbor windows in the database. When the tree is balanced this yields an O(logn) complexity for the search. This complexity was observed in our computations. SST is most effective for applications in which the target sequences show a high degree of similarity to the query sequence, such as assembling shotgun sequences or matching ESTs to genomic sequence. The algorithm is also an effective filtration method. Specifically, it can be used as a preprocessing step for other search methods to reduce the complexity of searching one large database against another. For the problem of identifying overlapping fragments in the assembly of 120 000 fragments from a 1.5 megabase genomic sequence, SST is 15 times faster than BLAST when we consider both building and searching the tree. For searching alone (i.e. after building the tree index), SST 27 times faster than BLAST. AVAILABILITY: Request from the authors.

Full Text

RESERVED.

AN 1999.0514804 PASCAL

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TIEN Markovian structures in biological **sequence alignments**

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SO Journal of the American Statistical Association, (1999), 94(445), 1.15, 44 refs.

ISSN: 0162.1459 CODEN: JSTNAL

DT Journal

BL Analytic

CY United States

LA English

AV INIST.3094, 354000083478830010

AB The **alignment** of multiple homologous biopolymer **sequences** is crucial in research on protein modeling and engineering, molecular evolution, and prediction in terms of both gene function and gene product structure. In this article we provide a coherent view of the two recent models used for multiple **sequence alignment**. the hidden Markov model (HMM) and the block-based motif model. to develop a set of new **algorithms** that have both the sensitivity of the block-based model and the flexibility of the HMM. In particular, we decompose the standard HMM into two components: the insertion component, which is captured by the so-called "propagation model," and the deletion component, which is described by a deletion **vector**. Such a decomposition serves as a basis for rational compromise between biological specificity and model flexibility. Furthermore, we introduce a Bayesian model selection criterion that. in combination with the propagation model, genetic **algorithm**, and other **computational** aspects. forms the core of PROBE, a multiple **alignment** and database search methodology. The application of our method to a GTPase family of protein **sequences** yields an **alignment** that is confirmed by comparison with known tertiary structures.

L5 ANSWER 45 OF 78 MEDLINE

Full Text

AN 2002064973 MEDLINE

DN 21650566 PubMed ID: 11791227

TI Local multiple alignment of numerical sequences: detection of subtle motifs from protein sequences and structures.

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SO GENOME INFORMATICS SERIES, (2001) 12 83.92.

Journal code: 9717234. ISSN: 0919.9454.

CY Japan

DT Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals

EM 200208

ED Entered STN: 20020125

Last Updated on STN: 20020820

Entered Medline: 20020819

AB This paper presents a new method to find motifs from multiple protein sequences and multiple protein structures. The method consists of two parts: quantification and local multiple alignment. In the former part, protein sequences and protein structures are transformed into sequences of real numbers and real vectors respectively. In the latter part, fixed length regions having similar shapes are located. A Gibbs sampling algorithm for sequences of real numbers/vectors is newly developed for finding common regions. The results of the comparison with a standard Gibbs sampling program show that the method is particularly useful when structural information is available.

L5 ANSWER 50 OF 78 MEDLINE

Full Text

AN 2002105924 MEDLINE

DN 21825953 PubMed ID: 11836217

TI Integrated gene and species phylogenies from unaligned whole genome protein sequences.

AU Stuart Gary W; Moffett Karen; Baker Steve

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SO BIOINFORMATICS, (2002 Jan) 18 (1) 100.8.

Journal code: 9808944. ISSN: 1367.4803.

CY England: United Kingdom

DT Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals

EM 200206

ED Entered STN: 20020212

Last Updated on STN: 20020611

Entered Medline: 20020610

AB MOTIVATION: Most molecular phylogenies are based on **sequence alignments**. Consequently, they fail to account for modes of **sequence** evolution that involve frequent insertions or deletions. Here we present a method for generating accurate gene and species phylogenies from whole genome **sequence** that makes use of short character string matches not placed within explicit **alignments**. In this work, the singular value decomposition of a sparse tetrapeptide frequency matrix is used to represent the proteins of organisms uniquely and precisely as **vectors** in a high-dimensional space. **Vectors** of this kind can be used to calculate pairwise distance values based on the angle separating the **vectors**, and the resulting distance values can be used to generate phylogenetic trees. Protein trees so derived can be examined directly for homologous **sequences**. Alternatively, **vectors** defining each of the proteins within an organism can be summed to provide a **vector** representation of the organism, which is then used to generate species trees. RESULTS: Using a large mitochondrial genome dataset, we have produced species trees that are largely in agreement with previously published trees based on the analysis of identical datasets using different methods. These trees also agree well with currently accepted phylogenetic theory. In principle, our method could be used to compare much larger bacterial or nuclear genomes in full molecular detail, ultimately allowing accurate gene and species relationships to be derived from a comprehensive comparison of complete genomes. In contrast to phylogenetic methods based on **alignments**, **sequences** that evolve by relative insertion or deletion would tend to remain recognizably similar.